DEVELOPMENT PROGRAM FOR D₂O LATTICE REACTIVITY CALCULATIONS

by

G. CASINI, A. KIND, G. ROSSI

1963

ORGEL Program
Joint Nuclear Research Center
Ispra Establishment - Italy
Reactor Physics Department
Applied Mathematical Physics

Paper presented at the Panel on Heavy Water Lattices
Vienna, 18-22.2.1963
LEGAL NOTICE

This document was prepared under the sponsorship of the Commission of the European Atomic Energy Community (EURATOM).

Neither the EURATOM Commission, its contractors nor any person acting on their behalf:

1° — Make any warranty or representation, express or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this document, or that the use of any information, apparatus, method, or process disclosed in this document may not infringe privately owned rights; or

2° — Assume any liability with respect to the use of, or for damages resulting from the use of any information, apparatus, method or process disclosed in this document.

This report can be obtained, at the price of Belgian Francs 25,— from:

Please remit payments:
— to BANQUE DE LA SOCIETE GENERALE (Agence Ma Campagne) — Brussels — account No 994.558,
— to BELGIAN AMERICAN BANK AND TRUST COMPANY — New York — account No 121.88,
— to LLOYDS BANK (Foreign) Ltd. — 10 Moorgate — London E.C.2.

giving the reference: "EUR 239 — Development Program for D2O Lattice Reactivity Calculations".

Printed by Guyot,
Brussels, April 1963.
The method used today at Euratom for reactivity evaluations of ORGEL type reactors is described in the paper: "A simplified method for organic, heavy water lattice calculations".

Following the requirements fixed by the general activity program of Euratom regarding this reactor type, a development of the method used is needed. The method necessary for the engineering work is not a recipe such as it could be used for industrial design purposes, but a method which must make possible a
satisfactory evaluation of the incidence on the kwhr price of very important design variations. Due to this fact, the right way seems not to be that of a further development in the direction of an empirical correlation recipe, but that of the development of a more “physical” method by which the elements entering in the reactivity determination are, as far as possible, physically analysed and carefully taken into account.

Our work is now going in two directions:

— the first one is that of analysing the interest of extensive numerical computations based on fundamental data. The presence at Ispra of important computation facilities may make this way interesting;

— the second one is that of trying to develop simplified methods which do not need high computation times but treat the essential points in a correct physical way.

An analysis of the interest of the two lines considered should be possible.

In this paper some particular problems studied in the framework of the second line of approach are analysed. The main ones are an improvement in the determination of the $p$ factor and a correct description of the space dependent neutron spectrum in the lattice. Both points are of particular importance for lattices with fuel element bundles of great dimensions and containing moderating coolant.
DEVELOPMENT PROGRAM FOR D₂O LATTICE REACTIVITY CALCULATIONS

by

G. CASINI, A. KIND, G. ROSSI

1963

ORGEL Program
Joint Nuclear Research Center
Ispra Establishment - Italy
Reactor Physics Department
Applied Mathematical Physics

Paper presented at the Panel on Heavy Water Lattices
Vienna, 18-22.2.1963
DEVELOPMENT PROGRAM FOR D\textsubscript{2}O
LATTICE REACTIVITY CALCULATIONS

SUMMARY

The method used today at Euratom for reactivity evaluations of ORGEL type reactors is described in the paper: "A simplified method for organic, heavy water lattice calculations".

Following the requirements fixed by the general activity program of Euratom regarding this reactor type, a development of the method used is needed. The method necessary for the engineering work is not a recipe such as it could be used for industrial design purposes, but a method which must make possible a satisfactory evaluation of the incidence on the kwh price of very important design variations. Due to this fact, the right way seems not to be that of a further development in the direction of an empirical correlation recipe, but that of the development of a more "physical" method by which the elements entering in the reactivity determination are, as far as possible, physically analysed and carefully taken into account.

Our work is now going in two directions:
— the first one is that of analysing the interest of extensive numerical computations based on fundamental data. The presence at Ispra of important computation facilities may make this way interesting;
— the second one is that of trying to develop simplified methods which do not need high computation times but treat the essential points in a correct physical way.

An analysis of the interest of the two lines considered should be possible.

In this paper some particular problems studied in the framework of the second line of approach are analysed. The main ones are an improvement in the determination of the p factor and a correct description of the space dependent neutron spectrum in the lattice. Both points are of particular importance for lattices with fuel element bundles of great dimensions and containing moderating coolant.

The method now in use at Euratom for reactivity evaluations of ORGEL type reactors (D\textsubscript{2}O moderated, organic cooled) is presented at this Symposium in the paper "A simplified method for organic, heavy water lattice calculations" (Ref. 1).

This method was born with a well-defined target: to put in a short time into the hands of the engineers in charge of the first ORGEL design evaluations a handy instrument for doing their reactivity calculations. This target was reached about six months ago. Since that time the activity of the Reactor Physics Department at Ispra in the field of D\textsubscript{2}O moderated reactors was directed towards a second goal, tightly connected with the more general Euratom programme in the line of this type of reactors.

First of all, after the initial step of a rough evaluation of the interest of D\textsubscript{2}O moderated and organic cooled reactors, the necessity was felt, in the framework of this reactor concept, for a more accurate evaluation of the influence of different widespread design variations on the end reactivity balance. Furthermore, the interest of Euratom with regard to D\textsubscript{2}O moderated reactors is now progressively spreading to other coolants.

To satisfy these new requirements, our present reactivity calculation method is no longer sufficient and a more accurate and powerful one is needed.

To continue along the line of a correlation recipe purely based on integral experiments would result in much too big an amount of such experiments, being as a result too expensive and time-consuming. Furthermore, the presence at Ispra since the beginning of 1962 of powerful
computation facilities renders the method of direct reactivity calculations on the basis of elementary nuclear data much more attractive for us than in the past. However, one must pay attention not to use guns to shoot flies. Some of the existing codes are unnecessarily powerful and therefore too heavy to get out of them reactivity results for D$_2$O reactors; furthermore, the existing uncertainties in the nuclear data make the so obtained results not completely reliable. The possibility exists of a very deep simplification in the computing effort and of a correct selection of the set of experimental data to be used if a preliminary accurate analysis is done of the physical characteristics of the lattices in question and of the use for which the calculation scheme is intended.

In view of these considerations, our line of action to get a suitable calculation instrument is the following:

No further work will be done to develop empirical correlation recipes in which, such as in Caroline I (Ref. 2), the adjustment parameters have mainly a formal meaning.

An extensive work is in progress to analyse the interest of developing more or less elaborate computational methods using, when needed, already existing codes.

An experimental programme is being elaborated to get the data needed as input into the calculation scheme and to verify its final validity.

As far as the sophisticated methods are concerned, a multigroup ORGEL lattice calculation, using the existing codes for IBM 7090, is now under study; the cell calculation is performed by the DSN code (Ref. 3); in the epithermal part the input cross sections for DSN are evaluated by the GAM-I code (Ref. 4). The self-shielding effects for U$_{238}$ absorption resonances are calculated by GAM-I by using the Adler et al. method (Ref. 5); a comparison of the results obtained by this method with the Hellstrand measurements for clusters of rods immersed in light water is in progress.

Concerning the development of a simplified method, different problems are arising according as one has to deal with the reactivity of clean cold lattices, temperature effects, or long term reactivity.

Regarding the clean cold lattices and as far as the up-to-date developed ORGEL fuel elements are concerned, Caroline I could in principle do the job. Nevertheless, some development work is needed to treat other fuel element designs, for instance 4 rod bundles, or other coolants.

Termidor (Ref. 6) describes in a fairly satisfactory way the temperature effects in D$_2$O cooled lattices. However, it is not yet clearly established how far this is the case for organic cooling.

As regards the long term reactivity calculations, due to the fact that the $p$ factor coming out of Caroline I has no clear physical meaning, we have no information on this way about the actual initial conversion factor. Furthermore, the well-known uncertainties in the cross-sections and in the $\eta$ values for the Pu isotopes, together with a lack of information on the dependence of the neutron spectrum on the irradiation of the fuel are such that the problem of the reactivity for irradiated lattices is far from being solved.

So, on the line of simplified methods, our theoretical work is going on with the following targets:

I. a better understanding of the assumptions made in Caroline I to calculate the fast fission factor.

The presence of the organic coolant in the fuel cluster produces a general softening of the spectrum in the fuel which enhances parasitic capture and reduces the fast fission factor by a slight amount. This effect is studied in a separate paper: "Fast neutron spectrum in ORGEL type reactors" (Ref. 7).
II. a more correct description of the resonance escape probability.

In Caroline I the p factor is written in the form:

\[ P = \exp \left( -\frac{V_i I_{\text{eff}}}{\xi_m \Sigma_m V_m + \xi_c \Sigma_c V_c} - P_B \right) \]

where, together with the usually employed symbols \( V, I_{\text{eff}}, \xi \) and \( \Sigma \), the suffixes f, m, c, mean respectively fuel, main moderator (D\textsubscript{2}O) and coolant (organic liquid and structural materials in the channel). The factor \( P_B \) is the advantage factor in the fuel obtained by assuming a single value for the resonance energy and by smearing out all materials over the cell.

By this way, three facts are not, or may not be, correctly taken into account:

1) the lattices considered have a fairly big pitch. So the introduction of only one advantage factor \( P_B \) may not take correctly into account the fact that different resonances, mainly those at high energies, should be put into the calculation with their advantage factors, which are increasing with the energy;

2) the heterogeneous cell structure could cause a sensible distortion in the flux shape as compared with the one calculated by means of an homogeneization;

3) the underestimation of the flux in which the organic liquid is placed as compared with D\textsubscript{2}O could bring a too high underestimation of the slowing-down power of the hydrogen in the fuel channel.

While on the basis of a rough two epithermal group evaluation point b) does not seem to introduce serious errors, points a) and c) need a more careful analysis. Point c) could for instance contribute to the discrepancies found (Ref. 1) between calculated and measured buckling in the cases of high hydrogen densities or big coolant volumes in the channel.

In order to solve in a simple way all these points the following procedure is being followed: to evaluate the flux distribution across the cell corresponding to the most important resonances of U\textsubscript{238} a multigroup collision probability code has been established. The resonance parameters for U\textsubscript{238} corresponding to the above-mentioned groups are introduced as effective resonance integrals according to the suggestion made by Brooks et al. (Ref. 8). For the other materials in the cell the group averaged microscopic cross sections are introduced once for all.

III. a more satisfactory description of the space energy distribution of the thermal neutron flux in the cell.

The improvements to the present calculation method as regards the thermal neutron flux distribution in the cell concern the following main points:

1) The epithermal contributions to the effective cross sections must be taken into account.

The most suggestive way seems to be on the line of the Horowitz and Tretiakoff procedure (Ref. 9). The well-known difficulties of the Westcott formalism are basically overcome by Horowitz and Tretiakoff; nevertheless some points require a careful analysis in view of practical purposes.

The complication due to the presence of moderating materials in the rod could be avoided in a simple manner on the basis of the hypothesis of independence between hardening and rethermalization (Ref. 10).
The problem of evaluating the ζ parameter (which describes the heterogeneity of the lattice) was analysed, by taking as reference a natural uranium heavy water reactor cell, for which the results of detailed space energy calculations and fine structure flux measurements are available (Ref. 11). Two ways are open: an evaluation by simple methods of the ratio \( \frac{N_n(x)}{N_m(x)} \) between thermal neutron densities in fuel and moderator as a function of energy, or the calculation by standard one-group methods of integral quantities depending on ζ (for instance the disadvantage factor).

The first way is strongly limited by the requirements of simplicity, whereas the second one seems to be at this moment the most promising.

2) The pure hardening effect must be included in the lattice calculations. Our running method is based on a very simple diffusion multigroup model (Ref. 12), which probably underestimates the hardening, due to the fact that a maxwellian shape of the spectrum is supposed in the moderator up to the interface between moderator and rod. On the other hand, an analysis of the Horowitz and Tretiakoff approximation for the ratio \( \frac{N_n(x)}{N_m(x)} \) seems to show that the \( h(x,z) \) function describes fairly well, as a simplified approach, the mean hardening of the thermal neutron spectrum in the fuel. Therefore, if this procedure is chosen, the problem of a simplified evaluation of the hardening in the fuel element should in principle be solved.

It may be of interest to point out that the functional dependence of the \( \frac{N_n(x)}{N_m(x)} \) ratio on x can be justified starting from the model of a purely absorbing body immersed in an isotropic neutron bath: this analysis shows in an interesting way the meaning and the limits of the Horowitz and Tretiakoff one-parameter approximation.

As regards the rethermalization effect, we are conscious that the two overlapping thermal group approximation is in a general way rather unsatisfactory, particularly close to the interface between the two media at different temperatures. On the other hand, the solution of the rethermalization problem with absorption in cylindrical geometry, also on the basis of the simple fundamental heavy gas - diffusion equation, would go out of the framework of simplified methods. Therefore, we do not intend to develop further simplified methods to solve this problem: as a matter of fact we dispose, if needed, of sophisticated methods to get a detailed space-energy description of the thermal neutron flux distribution in the cell (\( S_n \) multigroup, First Flight Collision Probability methods). We intend on the contrary to analyse more carefully the neutron transfer process between the two overlapping thermal groups, by taking into account the specific properties of the chemical binding in the organic molecules.

The experimental work intended to sustain the above-described theoretical programme is the following:

I — CLEAN COLD LATTICES

1) A series of thermal fine structure measurements in simple geometry natural uranium - heavy water - organic lattices has been performed during September 1962 in Aequilon II at Saclay (France). In these experiments the fuel element was a single uranium metal rod, 44 mm in diameter, surrounded by an organic liquid layer contained in an aluminum tube. The results of these measurements are given in Ref. 13. A second set of thermal fine structure measurements in an ECO type fuel element (the same as the one used in the experiments of effective resonance integral, see point 2 below) will be performed in Aequilon II during next spring.
2) Two series of measurements of the effective resonance integral in fuel elements is being performed in the Ispra I reactor by the Neutron Physics Service. The first set of experiments uses as fuel element a cluster of 12 rods of natural uranium, 12 mm in diameter, immersed in an organic liquid of the type which will be used as reference loading in the ECO reactor. The second set of experiments will use as fuel element a uranium carbide single rod, of diameter varying between 6 and 30 mm. These experimental results will be of a rather general interest because there are no data for uranium carbide available in the open literature.

3) Initial conversion factor measurements on typical fuel elements will be performed in the ECO facility.

4) A series of critical experiments will be performed in ECO, starting on the beginning of 1964. The first measurement will be done on UC fuelled lattices.

   The possibility of making complementary $K_\infty$ measurements is under study.

II — TEMPERATURE EFFECTS

1) Time of flight spectrum measurements in organic liquids are foreseen.

   A box containing organic liquid (polyphenyls) will be introduced in the thermal column of the Ispra I reactor. Uranium plates surrounding the box will provide a slowing-down source for the thermal neutron spectrum in the organic. A poison will be mixed to the organic liquid to have a distortion in the maxwellian shape. The description of this distortion depends on the theoretical model assumed for the interaction between slow neutrons and bound protons.

2) As a first possibility of selection between different types of scattering kernels and as an auxiliary measurement in view of the principal experiment, a series of transmission measurements on polyphenyls is already in progress.

3) At the same time, an information about the rotational freedom degrees of the polyphenyl molecules will be provided by measuring the energy change of cold neutrons scattered by organic samples.

4) Activation measurements with $1/v$ and non $1/v$ detectors are foreseen in ECO with different moderator and coolant temperatures.

5) A series of critical measurements with heated fuel channels is programmed for 1965 in ECO.

III — BURN-UP MEASUREMENTS

1) Activation measurements, mainly with Pu detectors, are planned to be made in ECO on fuel elements containing well-defined small quantities of Pu isotopes.

2) Oscillation experiments are also planned with the following fuel elements:
   a) containing small quantities of Pu isotopes,
   b) single irradiated rods to detect the fission products effect,
   c) bundles with radially varying Pu contents to simulate non-uniform burn-up.

   Concerning point a) a series of oscillation measurements, by using synthetic uranium-plutonium fuel elements will be performed in 1964 on the ECO reactor.

   The realization of the other two points is now under study.
REFERENCES


9 — J. HOROWITZ and O. TRETIAKOFF — Effective cross sections for thermal reactors — EANDC(E) 14 (1960).


